

Hexanoic acid, 5-oxo-, methyl ester

Other names:	Methyl 4-acetylbutyrate Methyl 5-oxohexanoate 5-Oxohexanoic acid methyl ester Methyl ester of 5-oxohexanoic acid
Inchi:	InChI=1S/C7H12O3/c1-6(8)4-3-5-7(9)10-2/h3-5H2,1-2H3
InchiKey:	AVVPOKSKJSJVIX-UHFFFAOYSA-N
Formula:	C7H12O3
SMILES:	<chem>COC(=O)CCCC(C)=O</chem>
Mol. weight [g/mol]:	144.17
CAS:	13984-50-4

Physical Properties

Property code	Value	Unit	Source
gf	-354.78	kJ/mol	Joback Method
hf	-545.19	kJ/mol	Joback Method
hfus	18.27	kJ/mol	Joback Method
hvap	47.08	kJ/mol	Joback Method
ie	9.60 ± 0.20	eV	NIST Webbook
log10ws	-0.90		Crippen Method
logp	0.919		Crippen Method
mcvol	118.500	ml/mol	McGowan Method
pc	3152.62	kPa	Joback Method
tb	489.72	K	Joback Method
tc	676.50	K	Joback Method
tf	290.74	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.79	J/molxK	489.72	Joback Method
cpg	304.37	J/molxK	645.37	Joback Method
cpg	295.47	J/molxK	614.24	Joback Method
cpg	286.16	J/molxK	583.11	Joback Method

cpg	276.45	J/mol×K	551.98	Joback Method
cpg	266.32	J/mol×K	520.85	Joback Method
cpg	312.87	J/mol×K	676.50	Joback Method
dvisc	0.0002983	Paxs	489.72	Joback Method
dvisc	0.0003773	Paxs	456.56	Joback Method
dvisc	0.0004951	Paxs	423.39	Joback Method
dvisc	0.0006804	Paxs	390.23	Joback Method
dvisc	0.0009920	Paxs	357.07	Joback Method
dvisc	0.0015623	Paxs	323.90	Joback Method
dvisc	0.0027292	Paxs	290.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13984504&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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